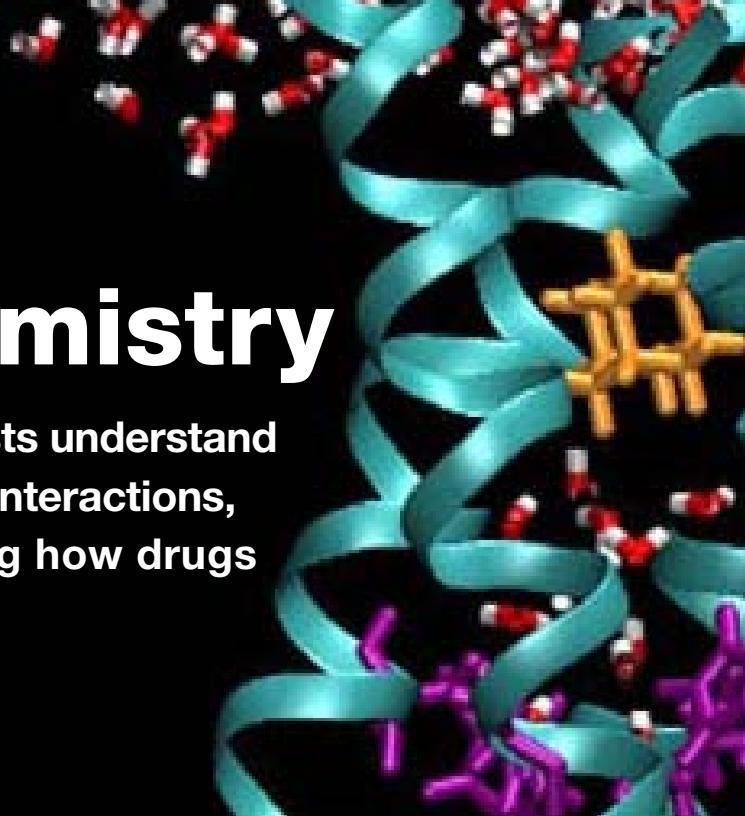


# Biochemistry

**OSG helps scientists understand water and protein interactions, possibly impacting how drugs are designed.**



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## Biochemistry

Scientists study the interactions between proteins and water to understand how water mediates drug-protein interactions.

Their findings may have a significant impact on the way future drugs are designed.

Ana Damjanovic, of the National Institutes of Health & Johns Hopkins University uses the Harvard-developed CHARMM application to model the structure and behavior of molecular systems.

"I'm running many different simulations to determine how much water exists inside proteins and whether these water molecules can influence the proteins," Damjanovic says.

OSG experts also helped Ana and her team develop easy-to-run workflow software for submitting jobs to the grid. The researchers were able to focus on science, not on the grid infrastructure.

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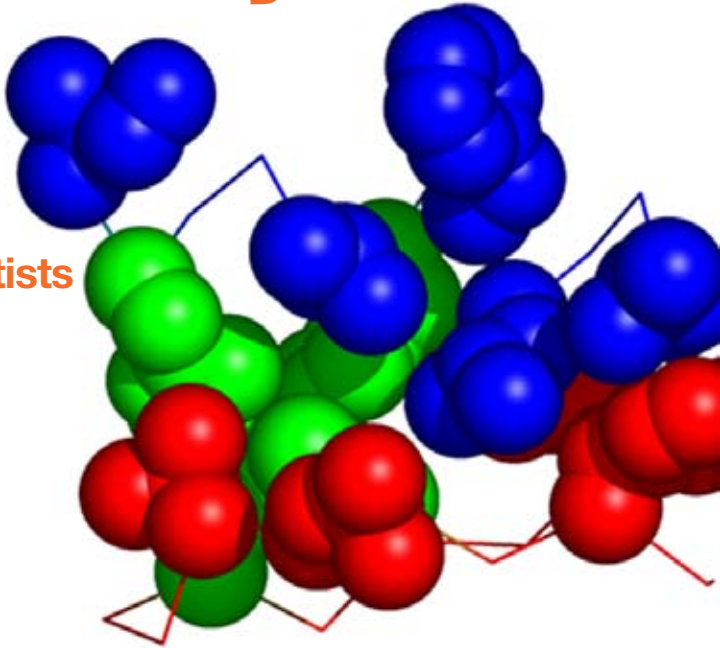


# Molecular Dynamics

OSG supports scientists  
searching for cures  
to serious disease.



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## Molecular Dynamics

Scientists are studying proteins in order to design good proteins that can mitigate bad, disease-promoting proteins. This could lead to new treatments and eventually cures for serious diseases, such as diabetes, Alzheimer's, HIV/AIDS and many cancers.

Brian Kuhlman, Head of the Kuhlman Laboratory in the UNC School of Medicine, is one such scientist. He uses the Rosetta application to sample different combinations of amino acid sequences and the proteins they form.

Kuhlman's small research lab is not able to muster the necessary 3,000 CPU hours that is consumed across 10,000 compute jobs for each protein in order to analyze the thousands of different ways it might fold.

Kuhlman has not yet designed his good protein, but he's closer than ever: "We've improved protein stability and binding affinity," he says. OSG has helped Kuhlman come a step closer to mitigating disease-causing proteins.

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# Coastal Modeling

**OSG enables meteorologists to  
run more climate models, resulting  
in more accurate forecasts.**



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1000

## Coastal Modeling

Heavy precipitation and stormy weather known as convective precipitation occurs during spring, summer and early fall as sea breezes combine with mountainous terrain. This type of precipitation is difficult to predict and requires fine-scale atmospheric modeling.

Brian Etherton and his colleagues in the Department of Meteorology at the University of North Carolina Charlotte are increasing the accuracy of these storm predictions. They use the Weather Research and Forecasting (WRF) system, a next-generation numerical weather predication system, to model space over the Carolinas under different physical conditions.

The OSG is being used to run ensembles of 16 different climate models to more accurately predict convective precipitation. The ensembles are differentiated by start time and a variety of physical parameterizations, such as air/surface exchanges of heat and moisture.

The result is a far more accurate forecast than a single model.

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# Gravitational-Wave Physics

**OSG matches LIGO data with idle time  
on individual computers worldwide  
to search for spinning neutron stars.**



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## Gravitational-wave Physics

Scientists at the Laser Interferometer Gravitational-Wave Observatory (LIGO) are trying to detect ripples in the fabric of space and time. It is thought that far-off astronomical events, such as the collision of two neutron stars, will produce these ripples. Their characteristics will give us detailed information about the event that took place.

Britta Daudert is the head of the LIGO-Grid application team at Caltech.

OSG Usage stats to come.

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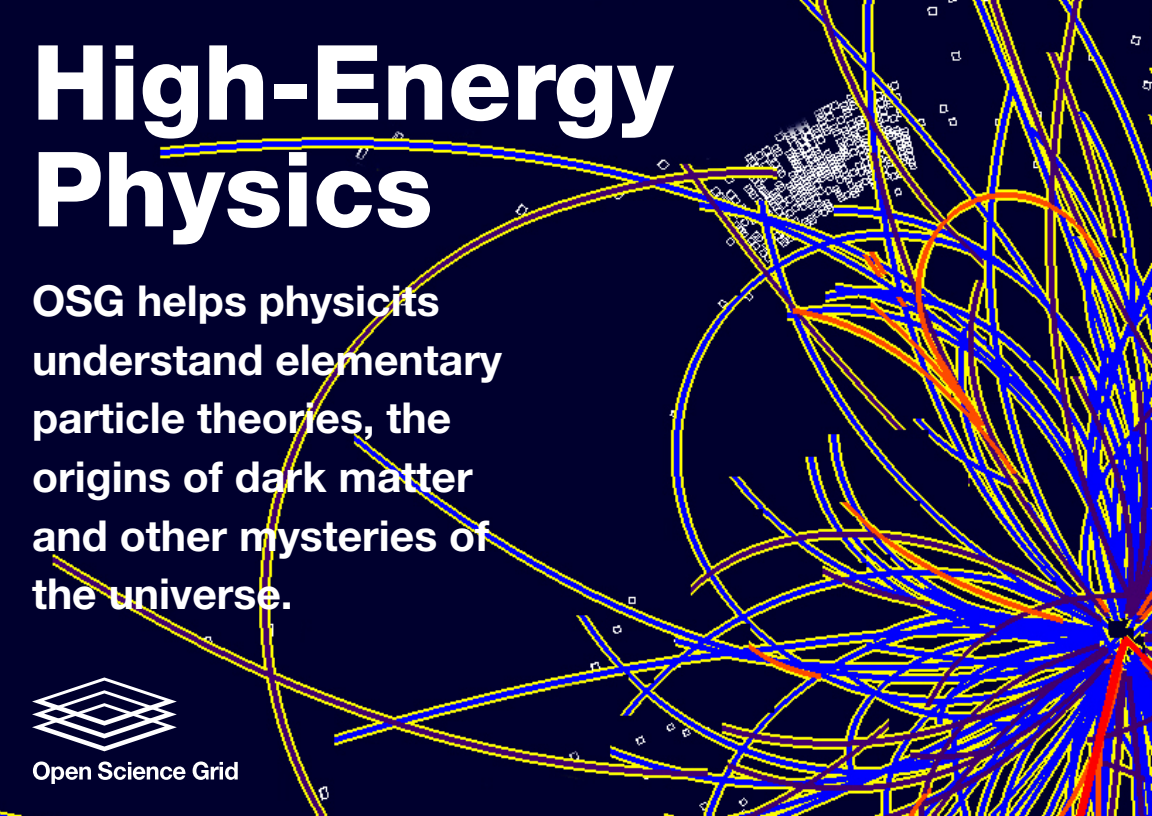


# High-Energy Physics

OSG helps physicists understand elementary particle theories, the origins of dark matter and other mysteries of the universe.



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## High-energy Physics

Scientists study elementary particle collisions at high energies in order to understand their characteristics. The results from such experiments improve our understanding of elementary particle theories, the origins of dark matter, and other mysteries of the universe.

Members of the LHC collaborations ATLAS and CMS use OSG to analyze their immense amount of data in order to obtain their results, relying on the OSG as the US infrastructure on which the Worldwide LHC Computing Grid (WLCG) depends.

OSG has provided ATLAS and CMS with 30% of their needed processing cycles.

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